```
=> d full his

     (FILE 'HOME' ENTERED AT 15:18:55 ON 19 DEC 2002)

     FILE 'REGISTRY' ENTERED AT 15:19:10 ON 19 DEC 2002
L1             2 SEA ABB=ON  PLU=ON  NITRILASE/CN
L2             1 SEA ABB=ON  PLU=ON  NITRILE HYDRATASE/CN
               D L1 1-2
               D L2

     FILE 'HCAPLUS' ENTERED AT 15:20:15 ON 19 DEC 2002

     FILE 'REGISTRY' ENTERED AT 15:20:32 ON 19 DEC 2002
               SET SMARTSELECT ON
L3             SEL PLU=ON  L1 1- CHEM :      11 TERMS
               SET SMARTSELECT OFF

     FILE 'HCAPLUS' ENTERED AT 15:20:32 ON 19 DEC 2002
L4           830 SEA ABB=ON  PLU=ON  L3

     FILE 'REGISTRY' ENTERED AT 15:20:36 ON 19 DEC 2002
               SET SMARTSELECT ON
L5             SEL PLU=ON  L2 1- CHEM :       7 TERMS
               SET SMARTSELECT OFF

     FILE 'HCAPLUS' ENTERED AT 15:20:36 ON 19 DEC 2002
L6           821 SEA ABB=ON  PLU=ON  L5
L7           821 SEA ABB=ON  PLU=ON  L4 (L) L6
L8           218 SEA ABB=ON  PLU=ON  L7 (L) ((MICROORGANISM/CT) OR MICROORGAN?
                 OR BACTER? OR EUBACTER?)
L9            17 SEA ABB=ON  PLU=ON  L8 (L) (DEFECT? OR INACTIV? OR REDU?)
L10           11 SEA ABB=ON  PLU=ON  L9 AND PD<19991026
```

=> d ibib ab 1-11

L10 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:704348 HCAPLUS
DOCUMENT NUMBER: 132:34820
TITLE: Thermostable nitrilase catalyzed production of nicotinic acid from 3-cyanopyridine
AUTHOR(S): Almatawah, Q. A.; Cowan, D. A.
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, University College London, London, UK
SOURCE: Enzyme and Microbial Technology (**1999**), 25(8-9), 718-724
CODEN: EMTED2; ISSN: 0141-0229
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A thermostable **nitrilase** produced by the thermophilic **bacterium** Bacillus pallidus Dac521 catalyzed the direct hydrolysis of 3-cyanopyridine to nicotinic acid without detectable formation of nicotinamide. The reaction conditions for nicotinic acid prodn. were optimized by using free **bacterial** cells. Temp. and pH optima were 60.degree.C and 8.0, resp., with no detectable mass transfer limitation at the highest cell loading. Under optimized conditions, 100% of the 3-cyanopyridine substrate could be converted to nicotinic acid at a conversion rate of 76 nmol/min/mg dry cell wt. Free **bacterial** cells were effective in converting 3-cyanopyridine at concns. of up to 0.3 M and the intracellular 3-cyanopyridinase stability was increased in the presence of the substrate at concns. of 0.2 and 0.3 M. Both 3-cyanopyridine and nicotinic acid inhibited the hydrolysis of 3-cyanopyridine at concns. greater than 0.2 M. Cells immobilized in calcium alginate beads retained 98% of initial activity and were more resistant to **inactivation**/inhibition than nonimmobilized cells at 60.degree.C. Calcium alginate immobilized cells used in a column bioreactor retained 100% of 3-cyanopyridinase activity for over 100 h and 10 h when continuously supplied with 0.1 M 3-cyanopyridine at 50.degree.C and 60.degree.C, resp. The conversion efficiencies of the bioreactors operated at 50.degree.C and 60.degree.C, at 100% 3-cyanopyridinase activity, were 104 mg (substrate)/g (cells)/h and 208 mg (substrate)/g (cells)/h, resp.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:120991 HCAPLUS
DOCUMENT NUMBER: 130:295593
TITLE: A new enzymic method of nitrile synthesis by Rhodococcus sp. strain YH3-3
AUTHOR(S): Kato, Yasuo; Ooi, Ryoko; Asano, Yasuhisa
CORPORATE SOURCE: Biotechnology Research Center, Faculty of Engineering, Toyama Prefectural University, Kosugi, Toyama, 939-0398, Japan
SOURCE: Journal of Molecular Catalysis B: Enzymatic (**1999**), 6(3), 249-256
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The substrate specificity of a novel aldoxime dehydratase from E-pyridine-3-aldoxime assimilating **bacterium**, Rhodococcus sp. strain YH3-3, was examd. The enzyme catalyzed a dehydration reaction of various aryl- and alkyl-aldoximes to form the corresponding nitriles, but did not act on arylalkyl- and substituted alkyl-aldoximes. Of various aldoximes tested, E-pyridine-3-aldoxime was the most suitable substrate for the enzyme. E-Pyridine-3-aldoxime analogs such as O-acetyl-E-pyridine-3-aldoxime, Z-pyridine-3-aldoxime, and E/Z-pyridine-3-aldehyde-hydrazone also acted as substrates and were converted to 3-cyanopyridine. Heat-treatment of the cells increased the accumulation of 3-cyanopyridine from E-pyridine-3-aldoxime because the nitrile degrading enzyme, **nitrile hydratase**, was

inactivated. Under the optimized reaction conditions (pH 7.0, 30.degree.C), various nitriles were synthesized from the corresponding aldoximes in preparative scales with heat-treated cells of the strain. This is the first report on the microbial synthesis of nitriles from aldoximes.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:607955 HCAPLUS
DOCUMENT NUMBER: 129:341025
TITLE: Biochemistry and biotechnology of mesophilic and thermophilic nitrile metabolizing enzymes
AUTHOR(S): Cowan, Don; Cramp, Rebecca; Pereira, Rui; Graham, Dan; Almatawah, Qadreyah
CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, University College London, London, WC1E 6BT, UK
SOURCE: Extremophiles (**1998**), 2(3), 207-216
CODEN: EXTRFI; ISSN: 1431-0651
PUBLISHER: Springer-Verlag Tokyo
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 70 refs. Mesophilic nitrile-degrading enzymes are widely dispersed in **bacteria** and lower orders of the eukaryotic kingdom. Two distinct enzyme systems, a **nitrilase** catalyzing the direct conversion of nitriles to carboxylic acids and sep. but cotranscribed **nitrile hydratase** and amidase activities, are now well known. **Nitrile hydratases** are metalloenzymes, incorporating FeIII or CoII ions in thiolate ligand networks where they function as Lewis acids. In comparison, **nitrilases** are thiol-enzymes and the 2 enzyme groups have little or no apparent sequence or structural homol. The hydratases typically exist as .alpha..beta. dimers or tetramers in which the .alpha.- and .beta.-subunits are similar in size but otherwise unrelated. **Nitrilases**, however, are usually found as homomultimers with as many as 16 subunits. Until recently, the 2 nitrile-degrading enzyme classes were clearly sepd. by functional differences, the **nitrile hydratases** being aliph. substrate-specific and lacking stereoselectivity, whereas the **nitrilases** were enantioselective and arom. substrate-specific. The recent discovery of novel enzymes in both classes (including thermophilic representatives) has blurred these functional distinctions. Purified mesophilic nitrile-degrading enzymes are typically thermolabile in buffered soln., rarely withstanding exposure to temps. above 50.degree. without rapid **inactivation**. However, operational thermostability is often increased by addn. of aliph. acids or by use of immobilized whole cells. Low mol. stability has frequently been cited as a reason for the limited industrial application of "**nitrilases**"; such statements notwithstanding, these enzymes have been successfully applied for more than a decade to the kiloton prodn. of acrylamide and more recently to the smaller-scale prodn. of nicotinic acid, R-(-)-mandelic acid, and S-(+)-ibuprofen. There is also a rapidly growing catalog of other potentially useful conversions of complex nitriles in which the regioselectivity of the enzyme coupled with the ability to achieve high conversion efficiencies without detriment to other sensitive functionalities is a distinct process advantage.

L10 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:311675 HCAPLUS
DOCUMENT NUMBER: 129:105736
TITLE: Screening of novel enzymes for the production of useful compounds
AUTHOR(S): Yamada, Hideaki
CORPORATE SOURCE: Department of Agricultural Chemistry, Kyoto University, Kyoto, 606, Japan
SOURCE: Studies in Organic Chemistry (Amsterdam) (**1998**), 53(New Frontiers in Screening for Microbial Biocatalysts), 13-17
CODEN: SOCHDQ; ISSN: 0165-3253
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 7 refs. Our lab. at Kyoto University has in the past forty years, carried out basic studies on the synthesis of various biol. and chem. useful compds., using new and novel microbial enzymes isolated from the screened **microorganisms**. These compds. are L-dopa (.beta.-tyrosinase); D-p-hydroxyphenylglycine, D-phenylglycine (hydantoinase); Et (R)-4-chloro-3-hydroxybutanoate (aldehyde **reductase**); acrylamide, nicotinamide (**nitrile hydratase**); acrylic acid, nicotinic acid (**nitrilase**); 6-hydroxynicotinic acid (hydroxylase); D-malic acid (maleate hydratase); D-pantoic acid (aldonolactonase); and theobromine (oxygenase). Based on the results of our basic studies in this field, we have developed new processes for the industrial prodn. of useful compds., so called "hybrid processes", incorporating many technologies in microbiol., enzymol., biochem., enzyme engineering, chem. engineering and org. chem. for the prodn. of useful compds.

L10 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:224324 HCAPLUS
DOCUMENT NUMBER: 126:208954
TITLE: Production of amidase/nitrilase from Rhodococcus rhodochrous and its use in acrylamide polymer manufacture
INVENTOR(S): Armitage, Yvonne Christine; Hughes, Jonathan
PATENT ASSIGNEE(S): Allied Colloids Limited, UK; Armitage, Yvonne Christine; Hughes, Jonathan
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9706248	A1	19970220	WO 1996-GB1951	19960809 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
AU 9667073	A1	19970305	AU 1996-67073	19960809 <--
AU 707650	B2	19990715		
EP 839190	A1	19980506	EP 1996-927143	19960809 <--
R: AT, BE, DE, DK, ES, FR, GB, IT, NL, SE, IE				
JP 11510392	T2	19990914	JP 1996-508251	19960809 <--
US 6146861	A	20001114	US 1998-11025	19980724

PRIORITY APPLN. INFO.:		
GB 1995-16346	A	19950809
GB 1996-6047	A	19960322
WO 1996-GB1951	W	19960809

AB An amidase or **nitrilase** is made by continuous culture under carbon limitation using a carbon source which includes, resp., either (a) an amide or amide precursor or (b) a nitrile or nitrile precursor. Thus, Rhodococcus rhodochrous NCIMB 40756 is cultured under steady-state culture at a diln. rate of 0.04 h-1 in the presence of 1.1 g/L acetamide to produce elevated levels of amidase activity (22 U/mg after 150 h culture). The amidase cultured under continuous conditions was particularly stable (only a 3.1% drop of 8 U/g in activity from 2 to 12 days) in comparison to the amidase produced by the batch-cultured **microorganism** which underwent a drop of 48 U/mg (56.5%) in the same period. The novel amidase, and the amidase made by the defined process, are effective for converting (meth)acrylate, for instance in or after the polymn. of the acrylamide. Amidase-active cells immobilized in crosslinked polyacrylamide beads catalyze the hydrolysis of acrylamide to produce ammonium acrylate. When the reactor acrylamide is **reduced** to 27 g/L, sufficient acrylamide soln is automatically added to the reactor to

raise the acrylamide concn. to 30 g/L. This automatic feeding procedure provides a specific yield of 660 g ammonium acrylate produced per g dry wt. cells after 22 days, and a specific amidase activity of 226 .mu.mol/min/g. The improved stability and overall productivity of the amidase enzyme allows removal of contaminating (meth)acrylate during the purifn. of polyacrylamide or acrylamide-contg. copolymers.

L10 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:1006858 HCAPLUS
DOCUMENT NUMBER: 124:53841
TITLE: Fermentative manufacture of amides from nitriles
INVENTOR(S): Ueki, Nobuhide; Myasaka, Kyoyuki; Morimoto, Hironori
PATENT ASSIGNEE(S): Mitsubishi Kagaku Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07265091	A2	19951017	JP 1994-61208	19940330 <--

AB Amides are manufd. by hydration of nitriles by treatment with microorganisms or their prepns. crosslinked with glutaraldehyde (I). Thus, Rhizobium sp. MCI2643 (FERM BP-3953) was aerobically cultured in a medium contg. glucose, polypeptone, yeast ext., urea, and salts at 30.degree. and pH 7.5 for 36 h. The mixt. was centrifuged, the cells mixed with aq. Na2SO4 contg. oleic acid (II), washed, treated with aq. I soln., incubated with aq. acrylamide (III) soln., and then treated with acrylonitrile at 15.degree. for 3 min to manuf. III. Nitrile hydratase had a half-life of 47 h vs. 0.22 h for controls treated in the absence of I and II.

L10 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:487960 HCAPLUS
DOCUMENT NUMBER: 115:87960
TITLE: Novel cyanide-hydrolyzing enzyme from Alcaligenes xylosoxidans subsp. denitrificans
AUTHOR(S): Ingvorsen, Kjeld; Hoejer-Pedersen, Birgitte; Godtfredsen, Sven E.
CORPORATE SOURCE: Novo Nordisk A/S, Bagsvaerd, DK-2880, Den.
SOURCE: Applied and Environmental Microbiology (**1991**), 57(6), 1783-9
CODEN: AEMIDF; ISSN: 0099-2240
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A cyanide-metabolizing **bacterium**, strain DF3, isolated from soil was identified as A. xylosoxidans denitrificans. Whole cells and cell exts. of strain DF3 catalyzed the hydrolysis of cyanide to formate and NH3 without forming formamide as a free intermediate. The cyanide-hydrolyzing activity was inducibly produced in cells during growth in cyanide-contg. media. Cyanate (OCN-) and a wide range of aliph. and arom. nitriles were not hydrolyzed by intact cells of A. xylosoxidans denitrificans DF3. Strain DF3 hydrolyzed cyanide with great efficiency. Thus, by using resting induced cells at a concn. of 11.3 mg (dry wt.) per mL, the cyanide concn. could be **reduced** from 0.97M (.apprx.25,220 ppm) to <77 nM .apprx.0.002 ppm) in 55 h. Enzyme purifn. established that cyanide hydrolysis by A. xylosoxidans denitrificans DF3 was due to a single intracellular enzyme. The sol. enzyme was purified .apprx.160-fold, and the 1st 25 N-terminal amino acids were detd. by automated Edman degrdn. The mol. wt. of the active enzyme (purity, >97% as detd. by amino acid sequencing) was estd. to be >300,000. The cyanide-hydrolyzing enzyme of A. xylosoxidans denitrificans DF3 was tentatively named cyanidase to distinguish it from known **nitrilases** (EC 3.5.5.1) which act on org. nitriles.

L10 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:550894 HCAPLUS

DOCUMENT NUMBER: 113:150894
TITLE: Manufacture of trans-4-cyanocyclohexanecarboxylic acid amide with Corynebacterium
INVENTOR(S): Oishi, Kazuhiko; Otsubo, Kazumasa
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02124096	A2	19900511	JP 1988-274423	19881101 <--

AB The title compd. (I), useful as an intermediate for ulcer-inhibiting cyanocyclohexanecarboxylic acid amide, is manufd. by incubating trans-1,4-dicyanocyclohexane (II) with a **nitrile hydratase**-contg. and amidase-**defective** Corynebacterium. Corynebacterium A68 (microbiol. properties are given) was cultured in a medium contg. yeast ext., sucrose, and salts at 28.degree. for 2 days, centrifuged, and the **bacteria** incubated with 40 g II in phosphate buffer at 30.degree. for 3.5 h to yield 37.1 g I.

L10 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:548647 HCAPLUS
DOCUMENT NUMBER: 113:148647
TITLE: Detoxification of cassava pulp using Brevibacterium sp. R312
AUTHOR(S): Legras, J. L.; Jory, M.; Arnaud, A.; Galzy, P.
CORPORATE SOURCE: Ec. Natl. Super. Agron. Montpellier, Montpellier, 34060, Fr.
SOURCE: Applied Microbiology and Biotechnology (**1990**), 33(5), 529-33
CODEN: AMBIDG; ISSN: 0175-7598
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Brevibacterium sp. strain R312 has an endocellular .beta.-glucosidase, a **nitrile hydratase**, and an amidase that can break down some cyanoglucosides. Nonsterile cassava pulp suspensions were fermented using this strain and 70%-80% **redn**. of nitrile compds., in particular cyanoglucosides and .alpha.-hydroxynitriles, was obsd. This type of **nitrile-hydratase**-active **microorganism** could be a soln. for the detoxification of cassava. Expts. conducted with the yeasts Candida molischiana and C. wickerhamii showed no improvement in detoxification.

L10 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:548044 HCAPLUS
DOCUMENT NUMBER: 111:148044
TITLE: Haloarylnitrile degrading gene, its use, and cells containing the gene
INVENTOR(S): Stalker, David
PATENT ASSIGNEE(S): Rhone-Poulenc Agrochimie, Fr.
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8900193	A1	19890112	WO 1988-EP588	19880704 <--
W: AU, BG, BR, DK, JP, KR, RO, SU				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8768984	A1	19870728	AU 1987-68984	19870105 <--
AU 611080	B2	19910606		
BR 8705281	A	19871222	BR 1987-5281	19870105 <--

JP 63502720	T2	19881013	JP 1987-500738	19870105 <--
JP 07095952	B4	19951018		
HU 47972	A2	19890428	HU 1987-911	19870105 <--
HU 209143	B	19940328		
US 4810648	A	19890307	US 1987-71146	19870708 <--
AU 8820719	A1	19890130	AU 1988-20719	19880704 <--
BR 8807609	A	19900529	BR 1988-7609	19880704 <--
EP 373173	A1	19900620	EP 1988-905798	19880704 <--
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 03505663	T2	19911212	JP 1988-505852	19880704 <--
IL 87001	A1	19940826	IL 1988-87001	19880706 <--
ES 2010763	A6	19891201	ES 1988-2134	19880707 <--
ZA 8804894	A	19900425	ZA 1988-4894	19880707 <--
CA 1339683	A1	19980224	CA 1988-571422	19880707 <--
CN 1031252	A	19890222	CN 1988-104173	19880708 <--
DD 284048	A5	19901031	DD 1988-330727	19880708 <--
DD 285922	A5	19910110	DD 1988-317745	19880708 <--
DK 9000028	A	19900302	DK 1990-28	19900105 <--

PRIORITY APPLN. INFO.:	US 1987-71146	19870708
	US 1986-817226	19860108
	US 1986-845662	19860328
	WO 1987-US44	19870105
	EP 1987-420005	19870107
	WO 1988-EP588	19880704

AB The gene for a **bacterial nitrilase** specific for 3,5-dihalogenated-p-hydroxybenzonitriles (e.g. bromoxynil) is cloned. The gene may be used to produce the **nitrilase** or to prep. herbicide-resistant plant cells and plants. The **nitrilase** gene was isolated from Klebsiella pneumoniae ozaenae found in bromoxynil-contaminated soil and cloned and expressed in E. coli. E. coli contg. a plasmid encoding an N-terminal truncated **nitrilase** produced an enzyme with increased Vmax and specific activity and **reduced** Km (for bromoxynil) relative to the native enzyme. Plasmid pN1, contg. the **nitrilase** gene inserted into an ocs cassette, was constructed and introduced into Agrobacterium tumefaciens for integration into the T-DNA of the Ti plasmid. Tobacco leaf disks were incubated with the recombinant A. tumefaciens and tobacco plants bromoxynil-resistant plants were regenerated from the transformed plant cells.

L10 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:	1981:138099 HCAPLUS
DOCUMENT NUMBER:	94:138099
TITLE:	Detoxification of jojoba meal by lactobacilli
AUTHOR(S):	Verbiscar, Anthony J.; Banigan, Thomas F.; Weber, Charles W.; Reid, B. L.; Swingle, R. Spencer; Trei, John E.; Nelson, Edward A.
CORPORATE SOURCE:	Anver Biosci. Design, Inc., Sierra Madre, CA, 91024, USA
SOURCE:	Journal of Agricultural and Food Chemistry (**1981**), 29(2), 296-302 CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Selected strains of Lactobacillus acidophilus and L. bulgaricus were found to grow well on jojoba seed meal and **reduce** the levels of simmondsin [51771-52-9] and other cyano toxicants. After standing for 21 days at 26.degree. on a 30% moisture jojoba meal, L. acidophilus 629 lowered total toxicant levels 95-98%. NH3 used in the process facilitated the detoxification. The lactobacilli apparently modify the cyano groups of the toxicants during their growth, thereby detoxifying the meal. This is the first time that lactobacilli of any species or strain have been reported to act on cyano groups, indicating the possible presence of a **nitrilase** [**9024-90-2**] in this food grade **microorganism**. In addn. to rendering jojoba meal nontoxic to mice, poultry, sheep, and cattle, the Lactobacillus treatment increases palatability of deoiled jojoba meal, which is otherwise poorly accepted in animal rations. The treatment of jojoba meal with a Lactobacillus resembles an ensilage process.

```
=> d his

     (FILE 'HOME' ENTERED AT 09:13:36 ON 19 DEC 2002)

     FILE 'HCAPLUS' ENTERED AT 09:14:01 ON 19 DEC 2002
                E CYANO/CT
                E E7+ALL
                E CARBOXYL/CT
                E E7+ALL
                E AMIDE/CT
                E E6+ALL
                E MICROORGANISM/CT
                E E3+ALL
L1         218643 S (CYANO GROUP/CT) OR (NITRILE GROUP/CT) OR CYANO? OR NITRILE?
L2         324540 S (CARBOXYL GROUP/CT) OR CARBOXYL?
L3         164603 S (AMIDE GROUP/CT) OR (AMIDO GROUP/CT) OR AMIDE? OR AMIDO?
L4         574393 S (MICROORGANISM/CT) OR MICROORGAN? OR BACTER? OR EUBACTER?
L5             39 S L1 (L) L2 (L) L3 (L) L4
L6              9 S L5 (L) (DEFECT? OR INACTIV? OR REDU?)
L7              7 S L6 AND PD<19991026
```

=> d ibib ab 1-7

L7 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:246832 HCAPLUS
DOCUMENT NUMBER: 124:342165
TITLE: Recent developments in the use of enzyme-catalyzed reactions in organic synthesis resulting from work at Exeter University
AUTHOR(S): Jenkins, Gareth N.; Roberts, Stanley M.; Turner, Nicholas J.
CORPORATE SOURCE: Dep. Chem., Univ. Exeter, Exeter, Devon, EX4 4QD, UK
SOURCE: Electronic Conference on Trends in Organic Chemistry [CD-ROM] (**1996**), Meeting Date 1995, Paper 4. Editor(s): Rzepa, Henry S.; Leach, Christopher; Goodman, Jonathan M. Royal Society of Chemistry: Cambridge, UK.
CODEN: 62TKAB
DOCUMENT TYPE: Conference; General Review
LANGUAGE: English
AB A review with 69 refs. Topics include (1) hydrolase-catalyzed hydrolyses of **carboxylic** acid esters and **amides**, phosphate esters, **nitriles**, and epoxides, and esterification and intramol. esterification reactions. (2) **Redn.** of ketones to secondary alcs using whole-cell systems of isolated dehydrogenases, and oxidn of alicyclic and arom. substrates using monooxygenases and dioxygenases in **bacteria** and fungi, including enzyme-catalyzed Baeyer-Villiger oxidns. (3) Carbon-carbon bond forming reactions, including aldol reactions and formation of optically active **cyanohydrins** and enzyme-catalyzed acyloin type reactions. And (4) future developments of biotransformations and the use of biocatalytic methods for the stereocontrolled prepn of important target structures are discussed.

L7 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:264542 HCAPLUS
DOCUMENT NUMBER: 122:81351
TITLE: Bicyclic amine derivatives of quinolones as single stereoisomers, useful as antimicrobials
INVENTOR(S): Takemura, Makoto; Kimura, Youichi; Matsuhashi, Norikazu
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 34 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 603887	A2	19940629	EP 1993-120802	19931223	<--
EP 603887	A3	19950426			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
CA 2112165	AA	19940626	CA 1993-2112165	19931222	<--
NO 9304753	A	19940627	NO 1993-4753	19931222	<--
JP 06239857	A2	19940830	JP 1993-323011	19931222	<--
JP 3268098	B2	20020325			
FI 9305830	A	19940626	FI 1993-5830	19931223	<--
AU 9352695	A1	19940707	AU 1993-52695	19931223	<--
AU 669948	B2	19960627			
US 5654318	A	19970805	US 1993-172233	19931223	<--
RU 2125046	C1	19990120	RU 1993-56853	19931223	<--
CN 1095068	A	19941116	CN 1993-121757	19931225	<--
CN 1037441	B	19980218			

PRIORITY APPLN. INFO.: JP 1992-346030 A 19921225
OTHER SOURCE(S): MARPAT 122:81351
AB Title compds. I [X1, X2 = halo; R1 = H, OH, SH, halomethyl, alkyl, alkoxy, (un)substituted amino; R2 = certain (un)substituted bicyclic heterocyclic amino groups; A = N, CX3; X3 = H, halo, **cyano**, CF3, alkyl, alkoxy, (un)substituted amino; R = H, Ph, CH2OAc, CO2Et, alkyl,

alkoxymethyl, phenylalkyl, etc.] and salts are disclosed. The compds., and particularly those with a single stereoisomerism in the bicyclic amino group R2 and/or in the 1,2-cis-halocyclopropyl group, exhibit potent antimicrobial activity and also high safety due to **reduced** lipophilicity. For example, cis-2-fluorocyclopropanecarboxylic acid was resolved via diastereomeric **amides**, and the (+)-isomer was converted in several steps to (1R,2S)-(-)-8-chloro-6,7-difluoro-1-(cis-2-fluoro-1-cyclopropyl)-4-oxo-1,4-dihydroquinoline-3-**carboxylic** acid (II). Then, 2,3-pyridinedicarboxylic acid was converted in 8 steps to (S,S)-1-(tert-butoxycarbonyl)octahydropyrrolo[3,4-b]pyridine (III). Reaction of II with III in refluxing MeCN in the presence of Et3N, and deprotection with CF3CO2H, gave title compd. IV. The partition coeff. of IV in a CHCl3/phosphate buffer (pH 7.4) system was 6.69, vs. 35.8 for its structural analog BAY-Y 3118, which lacks the F atom on the cyclopropyl substituent. The MIC values of IV against 12 **bacterial** strains ranged from .ltoreq. 0.003 .mu.g/mL against Escherichia coli NIHJ, to 0.10 .mu.g/mL against Streptococcus faecalis.

L7 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:150832 HCAPLUS
DOCUMENT NUMBER: 116:150832
TITLE: Some recent developments in the use of enzyme catalyzed reactions in organic synthesis
AUTHOR(S): Roberts, Stanley M.; Turner, Nicholas J.
CORPORATE SOURCE: Dep. Chem., Univ. Exeter, Exeter/Devon, EX4 4QD, UK
SOURCE: Journal of Biotechnology (**1992**), 22(3), 227-44
CODEN: JBITD4; ISSN: 0168-1656
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with .apprx.75 refs. The following processes are discussed; enzyme-catalyzed hydrolyses of **carboxylic** acid esters and **amides**, phosphate esters, **nitriles** and epoxides; esterification and inter-esterification reactions catalyzed by enzymes; **redn**. of ketones to secondary alcs. using whole-cell systems or isolated dehydrogenases; oxidn. of alicyclic and arom. substrates using mono-oxygenases and dioxygenases in **bacteria** and fungi including enzyme-catalyzed Baeyer-Villiger oxidns.; aldol reactions; formation of optically active **cyanohydrins** and enzyme-catalyzed acyloin type reactions. The use of these biocatalytic methods for the stereocontrolled prepn. of important target structures and some of the future directions for the biotransformation area are discussed.

L7 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:474187 HCAPLUS
DOCUMENT NUMBER: 79:74187
TITLE: Certain derivatives of 3-aminopyrazole-4-carboxylic acid as potential antimetabolites of 4(5)-aminoimidazole-5(4)-carboxamide in microorganisms
AUTHOR(S): Zidarova, M. K.; Golovinski, E. V.; Maneva, L. S.
CORPORATE SOURCE: Inst. Biokhem., Sofia, Bulg.
SOURCE: Doklady Bolgarskoi Akademii Nauk (**1973**), 26(3), 419-22
CODEN: DBANAD; ISSN: 0366-8681
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three analog-antagonists of 4(5)-aminoimidazole-5(4)carboxamide (I) [360-97-4], 3-amino-4-carbethoxypyrazole (II) [6994-25-8], 3-mino-4-pyrazolecarboxylic acid (III) [41680-34-6], and 3-amino-4-pyrazolecarboxylic hydrazide (IV) [41621-10-7], substantially inhibited the growth of at least one of the following Gram-pos. **microorganisms**, Sarcina lutea, Bacillus subtilis, Staphylococcus aureus, the UV-2 and UV-3 respiration **defect** mutants of St. aureus and Neurospora crassa. II, III, and IV were ineffective against the Gram-neg. Escherichia coli, Pseudomonas aeruginosa, Candida tropicalis, and Proteus vulgaris; while 3-amino-4-**cyanopyrazole** [16617-46-2], 3-amino-pyrazole-4-carboxamide [5334-31-6], and 3-amino-4-pyrazole-**carboxylic** acid-**amidotin** [41621-12-9] were ineffective against all 10 **microorganisms**.

Inhibition by II, the least effective of II, III, and IV, against N. crassa could not be counteracted by .leq.50 .mu.m/ml I. All 6 derivs. of pyrazole had no antitumoral effect on Ehrlich's ascitic carcinoma in vitro.

L7 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1963:32964 HCAPLUS
DOCUMENT NUMBER: 58:32964
ORIGINAL REFERENCE NO.: 58:5530e
TITLE: Synthesis of cyclooctane carboxylic acids, their amides and alcohols
AUTHOR(S): Saharia, G. S.; Tyagi, M. P.
CORPORATE SOURCE: Univ. Delhi
SOURCE: J. Sci. Ind. Res. (India) (**1962**), 21B, 504
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Cyclooctane **carboxylic** acids (I) were synthesized as potential **bactericides** by the condensation of cyclooctanone with NCCH2CO2Et in the presence of AcONH4 and glacial HOAc; Et cyclooctylidenecyanoacetate (II) thus obtained furnished on **redn.**, Et cyclooctyl-.alpha.-**cyanoacetate** (III, R = H), which on condensation with alkyl and aryl halides and halo ethers, in the presence of NaOEt yielded III (R = Me, Et, allyl, CH2CO2Et, (CH2)2CO2Et, CH2Ph, CH2CHMeCO2Et). III on subsequent hydrolysis gave the resp. I. **Amides** and alcs. of I were prepd. in the usual manner.

L7 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1948:21372 HCAPLUS
DOCUMENT NUMBER: 42:21372
ORIGINAL REFERENCE NO.: 42:4579d-i
TITLE: 4-Pyridine derivatives
AUTHOR(S): Prijs, B.; Lutz, A. H.; Erlenmeyer, H.
CORPORATE SOURCE: Univ. Basel, Switz.
SOURCE: Helv. Chim. Acta (**1948**), 31, 571-7
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Interest in compds. affecting the growth of **microorganisms** led to a preliminary investigation of the possibility of prepg. 4-pyridineacetic acid from 4-pyridinemethanol (I) through the corresponding Br and CN derivs. Isonicotinic acid (10 g.), prepd. according to Wibaut and Ahrens (C.A. 35, 5894.5) from 4-ethylpyridine, was converted into the corresponding acid chloride-HCl, refluxed in 50 cc. abs. MeOH, and neutralized with 2 N Na2CO3. Extn. with ether and redistn. in vacuo of the crude residue of evapn. yielded 80% of the known Me isonicotinate, b15 100.degree.. The corresponding **amide**, m. 153-5.degree., was converted according to Camps (Arch. Pharm. 240, 368 (1902)) with P2O5 at 160-80.degree. and 25 mm. for several hrs. into ,55% of the **nitrile**, m. 79.degree. (picrate, m. 230.degree. (decompn.)). **Reduction** of 5 g. **nitrile** in 100 cc. MeOH (satd. with NH3 at 0.degree.) in the presence of Raney Ni prepd. according to Mozingo (C.A. 37, 4693.5) 4 hrs. at 70.degree. with H at 85 atm. gave 70% sirupy 4-aminomethylpyridine (II), b12 120-5.degree. (picrate, m. 179-80.degree. (decompn.)), converted by KCNO to 1-(4-pyridylmethyl)urea, C7H9N3O, m. 190-2.degree.. Treatment of 3.5 g. II in 75 cc. of 0.5 N HCl with freshly pptd. AgNO2 (from 7 g. AgNO3 and excess NaNO2), extn. of the product with ether, and working up gave 65% I, b12 140-2.degree., m. 41.degree. (picrate, m. 165-6.degree.). Better yields of I can be obtained more quickly by the desulfurization of Me thiolisonicotinate (III), m. 50-1.degree., b14 120-2.degree. (picrate, m. 145-6.degree.), prepd. by the action of MeSH on isonicotinyl chloride. Raney Ni (15 g.) in 200 cc. alc. (prereduced according to Mozingo) was stirred with 3.45 g. III until desulfurization by loss of H2S was complete. Distn. in vacuo of the oily product gave 93% I, identical with the previously prepd. compd. Investigations using I as starting material were discontinued when it was found that 2-phenyl-4-pyridineacetic acid (IV) could be prepd. by treating 4-picoline (V) with LiPh and **carboxylating** the addn. product with CO2. V (21 g.) was added to LiPh (prepd. from 3.2 g. Li according to Wittig, C.A. 35, 7938.6), and the reaction mixt. was refluxed 10 hrs. After cooling, a large excess of

solid CO2 was added in small portions. Working up gave 3.5 g. (16%) yellow product, recrystd. from alc. to colorless crystals of IV, C13H11NO2, m. 243-6.degree.; Me ester, m. 78-9.degree..

L7 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1937:41440 HCAPLUS
DOCUMENT NUMBER: 31:41440
ORIGINAL REFERENCE NO.: 31:5802i,5803a-i,5804a-i,5805a-b
TITLE: Acridine compounds produced in the development of the chemotherapeutic remedies of the 9-aminoacridine series
AUTHOR(S): Eisleb, O.
SOURCE: Med. u. Chem., Abhandl. med.-chem. Forschungsstatten I. G. Farbenind. (**1936**), 3, 41-59
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB A review of development of new antiseptic acridine derivs. based on the tissue-antiseptic trypaflavine is given. The previously used general methods for the prepn. of acridine compds. were Bernsthen's procedure of condensing HNPh2 with **carboxylic** acids in the presence of ZnCl2, etc., and the formation of acridones from diphenylamine-2-**carboxylic** acids by H2SO4 according to Graebe or with PCl5 and AlCl3 according to Ullmann. By Bernsthen's method, followed by pptn. of the acid sulfate and coloring matters with 10% H2SO4, pure 9-methylacridine (I) m. 117-18.degree., was prepd. Aq. solns. of the HCl salt (1:5000) are fatal to streptococci in vitro. A mixt. of 50 g. I with 100 cc. of 40% HCHO and 50 cc. alc. was boiled with stirring for 10 min. H2O was added to the cooled mixt. and the solid brown addn. product was filtered off, washed and taken up in hot MeOH. The addn. of 100 cc. H2O gave 53 g. of 9-.beta.-hydroxyethylacridine (II), C15H13NO, m. 154.degree.; HCl salt, m. 235.degree. (decompn.), with a lethal concn. of 1:500 to 1:4000 against various strains of streptococci. Boiling in AcOH in the presence of dry HCl for 30 min. converted II into Et acridyl-9-acetate, m. 120.degree., forming a HCl salt with streptococcidal lethal concn. 1:2000. Heating 1 part II with 5 parts of 66% HBr in a bomb-tube at 160-70.degree. gave quant. yields of 9-bromoethylacridine-HBr lethal concn.>1:2000, converted by trituration with Na2CO3 and crystn. from CCl4 into the free base (III), m. above 200.degree. (decompn.). Warming with secondary bases converted III into 9-[.beta.-(ethanolmethylamino)ethyl]acridine, isolated as the di-HCl salt, C18H22Cl2N2O, lethal concn. in vitro 1:8000, and 9-(.beta.-piperidinethyl)acridine, m. 137.5.degree.; diglycolate, C24H31N2O6, lethal concn. 1:30,000. Aq. solns. of the salts of these aminoethylacridines are unstable and the di-HCl salts liberate free HCHO on boiling in H2O. Condensation of I with p-ONC6H4NMe2 in alc. gave 85% of the anil (IV). A mixt. of 250 cc. HCl (d. 1.19) and 200 g. IV in 500 cc. H2O was heated. on the steam bath with stirring. The cool soln. gave bright yellow crystals which were washed in a mixt. of 1 part satd. NaCl soln. and 3 parts 2 N HCl and then dissolved in 2 l. of hot H2O. The addn. of 300 cc. 2 N NaOAc pptd. the free aldehyde which was washed and dried over H2SO4, yielding 82% (105 g.) of acridine-9-aldehyde (V), m. 150.degree.; HCl salt, lethal concn. 1:8000. V was **reduced** in concd. HCO2H with Zn dust treated with Cu to I. II was converted with H2NMe and H2NCH2CH2OH in alc. to the corresponding methylimine, m. 160.degree., and ethanolimine, which could not be **reduced** by the usual methods. A cold, well-stirred mixt. of 40 g. V, 200 g. abs. alc. and 14 g. MeNO2 was treated dropwise with MeONa prepd. from 5 g. Na in 60 cc. MeOH below 8.degree.. The thick reaction mixt. was dild. with 400 cc. H2O and filtered. Acidification of the filtrate with AcOH gave 40 g. of 9-(.omega.-nitro-.alpha.-hydroxyethyl)acridine, C15H12N2O3, m. 170.degree. (decompn.), which could not be **reduced** to the corresponding amino compd. V was smoothly converted into the corresponding secondary alcs. by treatment with alkyl Mg halides. The addn. of MeMgI from 7.5 g. Mg, 45 g. MeI and 100 g. Et2O to 41.4 g. V in 200 g. benzene gave, after decompn. with NH4Cl and the usual procedures, 42 g. of 9-.alpha.-hydroxyethylacridine (VI), C15H13NO, m. 178-80.degree.; HCl salt, difficultly sol. in H2O with lethal concn. >1:1000. Similarly were prepd. 9-.alpha.-hydroxypropyl- and 9-.alpha.-hydroxybutyl-acridine, m. 158-9.degree. and 121.degree. resp. The reaction of a Grignard soln. from 40 g. p-BrC6H4OEt, 4.8 g. Mg and 100

g. Et2O with 20.7 g. V gave the difficultly sol. acridyl-9-p-ethoxyphenylcarbinol, C22H19NO2, m. 202.degree.. By heating with 5 parts of 60% HBr in a bomb-tube at 160-70.degree., V was converted into 9-.alpha.-bromethyl-acridine-HBr, which reacted with MeNHCH2CH2OH to give the oily base, 9-[.alpha.-(ethanolmethylamino)ethyl]acridine, yielding a cryst. di-HCl salt, C20H28Cl2N2O2, contg. 1 mol. alc. of crystn. Oxidatio n of 45 g. VI in 200 g. of 50% H2SO4 by the addn. of CrO3, treatment with 750 cc. of 2 N NaOH and pptn. with 500 cc. of 2 N AcONa followed by recrystn. from CCl4, produced 9-acridyl Me ketone (VII), C15H11NO, m. 109.degree., converted into the isonitroso deriv. by stirring a cold mixt. of 11 g. VII, 6 g. iso-AmNO2 and 20 g. alc. with NaOEt from 40 g. alc. and 2.3 g. Na for 2 hrs. below 30.degree.. Ice was added and the alk. soln. was extd. with Et2O and then acidified with AcOH. The washed yellowish cryst. ppt. was dried in vacuo over H2SO4 and produced 6 g. of 9-acridyl isonitrosomethyl ketone which could not be **reduced** to 9-(.omega.-amino-.alpha.-hydroxyethyl)acridine. A soln. of 11 g. VII in 200 cc. of 40% HBr was heated for 15 min. on the steam bath with 3 cc. Br. The cold soln. was filtered and the crystals were washed with HBr, alc. and Et2O, giving 17 g. of 9-acridyl .omega.-bromomethyl ketone-HBr. A soln. of 163 g. IV in 1.5 l. of 25% H2SO4 was heated on the steam bath with stirring for 30 min. The resulting H2SO4 salt was washed and taken up in 300 g. concd. H2SO4, oxidized with CrO3 and pptd. with H2O. Purification of the ppt. by soln. in dil. NH4OH and pptn. from the filtered soln. with HCl gave 90 g. of pure acridine-9-**carboxylic** acid converted by refluxing with 4 parts of SOCl2 into the acid chloride which on treatment with various alcs. gave the following esters: Me, m. 127-8.degree.; Et .beta.-diethylaminoethyl-HCl, C20H22ClN2O2, m. 190-1.degree.. Treatment of the Et ester with H2NNH2 yielded the hydrazide, m. 244.degree., which was converted in 50% AcOH by treatment with NaNO2 in the cold into the azide, readily decompd. All attempts to obtain nuclear-substitution products of I were unsuccessful. The presence of an alkoxy group in the acridine nucleus was desirable and 3 methods for synthesizing 3-ethoxy-9-methylacridine, m. 139-40.degree., were worked out but were too laborious for further development. A generalization of Graebe's acridone synthesis by which substituted diphenylamine-2-**carboxylic** acids were converted into 9-chloroacridine (VIII) is discussed (cf. Borsche, Runge and Trautner, C. A. 27, 5744). The mobility of the 9-Cl group is greatest in 2-or 4-and 5-or 7-neg.-substituted derivs. and particularly with NO2-substituted acridines. Substitution in the 3-position has less effect on the mobility which is hindered by alkoxy-group substitution. Replacement of the 9-Cl group by reaction with AcCHNaCO2Et, NaCH(CO2Et)2, NaCN, etc. was successful with VIII and 3-amino-9-chloracridine but failed with the 2-alkoxy-9-chloroacridines, and also with 2-ethoxy-9-bromoacridine. A mixt. of NaOEt from 34.5 g. Na and 600 cc. alc. with 195 g. AcCH2CO2Et and 213.5 g. VIII was refluxed for 20 hrs. and, after cooling, was acidified with 1200 cc. of 2 N HCl. After 24 hrs. the yellow HCl salt was collected, washed with dil. HCl suspended in 2 l. H2O, and treated with excess Na2CO3. The dry reddish cryst. powder was recrystd. from 700 cc. alc., yielding 204 g. of Et acridyl-9-acetoacetate, C19H17NO3, m. 130.degree., cleaved by boiling with dil. H2SO4 to acridyl-9-acetone, C16H13NO, m. 146.degree.. Heating a mixt. of 100 g. VIII with 28 g. finely powd. NaCN in 400 cc. MeOH for 6 hrs. at 140-50.degree. in a closed pressure vessel with stirring gave 85 g. of crude olive-green needles which, on recrystn. from iso-AmOH, yielded faintly yellowish cryst. 9-**cyanoacridine** (IX), C14H8N2, m. 183.degree., **reduced** catalytically in pyridine in the presence of Pd on CaCO3 to 9-**cyanoacridane**. The Cl atom in VIII and its substitution products was readily replaced by NH2 and substituted amino groups at 130-40.degree.. With manifold neg. substituted groups and particularly in reactions with secondary bases the stability of the 9-substituent is so small that acridones were readily formed by the hydrolytic cleavage of the salts. The HCl salt of 9-aminoacridine (X) has a lethal concn. at 1:180,000, comparable with that of trypaflavine in contrast to the above-mentioned acridine derivs. The variation of the antiseptic power of X by the introduction of further substituents was studied by the prepn. and pharmacolog. testing of 200 new compds. and a list of compds. in which the NH2 group was modified is given. It was found that the introduction of alkoxy groups into the 1,8-positions of these compds. had a favorable influence on the **bactericidal**

properties but a real advance was made by the introduction of a further NH2 group in the 3- or 6-position. Rivanol, 2-ethoxy-6,9-diaminoacridine lactate, has been introduced into chemotherapy on account of its high antiseptic value against strepto- and staphylococci. The introduction of a 2nd amino group in a side chain also provides good **bactericidal** agents, particularly in substitution in the 3- or 6-nitro-9-aminoacridines which have proved to have healing value in total sepsis in animal tests. The compds. 2-ethoxy-6-nitro-9-(.beta.-diethylaminoethyl)aminoacridine, 2-.beta.-diethylaminoethoxy-6-nitro-9-aminoacridine, 2-ethoxy-6-nitroacridyl-9-aminoacet(.beta.-diethylaminoethyl) **amide** and 2,3-dimethoxy-6-nitro-9-(.gamma.-diethylamino-.beta.-hydroxypropyl)aminoacridine (No. 3582) are quoted as examples of 70 new substances of this type. The outstanding **bactericidal** power of No. 3582 is used in a mixt. with rivanol under the name entozon in veterinary medicine since it has been found that these NO2 derivs. have uncertain action in man. The falsity of argument by analogy in chemotherapeutic investigation is pointed out and it is stressed that series investigation provides the broadest basis on which to devise and choose substances with true optimal effect as medicinal remedies.

=> d l1 1-2

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2002 ACS
RN 82391-37-5 REGISTRY
CN Hydratase, nitrile (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Cyanopyridine hydratase
CN Acrylonitrile hydratase
CN Aliphatic nitrile hydratase
CN E.C. 4.2.1.84
CN **Nitrilase**
CN Nitrile hydratase
MF Unspecified
CI MAN
LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CEN, CHEMINFORMRX, CIN, EMBASE, PROMT, TOXCENTER, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
373 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
378 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L1 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2002 ACS
RN 9024-90-2 REGISTRY
CN **Nitrilase (9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Acetonitrilase
CN Benzonitrilase
CN E.C. 3.5.5.1
MF Unspecified
CI MAN
LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, EMBASE, PROMT, TOXCENTER, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
310 REFERENCES IN FILE CA (1962 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
313 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> d l2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 82391-37-5 REGISTRY
CN Hydratase, nitrile (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Cyanopyridine hydratase
CN Acrylonitrile hydratase
CN Aliphatic nitrile hydratase
CN E.C. 4.2.1.84
CN Nitrilase
CN **Nitrile hydratase**
MF Unspecified
CI MAN
LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CEN, CHEMINFORMRX, CIN, EMBASE, PROMT, TOXCENTER, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
373 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
378 REFERENCES IN FILE CAPLUS (1962 TO DATE)

NiceZyme View of ENZYME: EC 3.5.5.1

Official Name

Nitrilase.

Alternative Name(s)

None.

Reaction catalysed

```
    A nitrile
 +  H(2)O
<=>
    a carboxylate
 +  NH(3)
```

Comments

- Acts on a wide range of aromatic nitriles including (indole-3- yl)-acetonitrile and also on some aliphatic nitriles, and on the corresponding acid amides (cf. EC 4.2.1.84).

Cross-References

PROSITE	PDOC00712
BRENDA	3.5.5.1
EMP/PUMA	3.5.5.1
WIT	3.5.5.1
KYOTO UNIVERSITY LIGAND CHEMICAL DATABASE	3.5.5.1
IUBMB Enzyme Nomenclature	3.5.5.1
MEDLINE	Find literature relating to 3.5.5.1
SWISS-PROT	P32961, NRL1_ARATH; P32962, NRL2_ARATH; P46010, NRL3_ARATH; P46011, NRL4_ARATH; Q42965, NRL4_TOBAC; P33036, NRLA_ACISP; P20960, NRLA_ALCFA; P10045, NRLB_KLEPO;

View entry in original ENZYME format

If you would like to retrieve all the SWISS-PROT entries referenced in this entry, click here.

NiceZyme View of ENZYME: EC 4.2.1.84

Official Name

Nitrile hydratase.

Alternative Name(s)

Nitrilase.

Reaction catalysed

```
    An aliphatic amide
<=>
    a nitrile
 +  H(2)O
```

Comments

- Acts on short-chain aliphatic nitriles, converting them into the corresponding acid amides.
- Does not act on these amides or on aromatic nitriles (cf. EC 3.5.5.1).

Cross-References

BRENDA	4.2.1.84
EMP/PUMA	4.2.1.84
WIT	4.2.1.84
KYOTO UNIVERSITY LIGAND CHEMICAL DATABASE	4.2.1.84
IUBMB Enzyme Nomenclature	4.2.1.84
MEDLINE	Find literature relating to 4.2.1.84
SWISS-PROT	P21219, NHA1_RHORH; P29378, NHA2_RHORH; P27764, NHAA_PSECL; P97051, NHAA_PSEPU; P13448, NHAA_RHOER; Q53118, NHAA_RHOSO; P27763, NHAB_PSECL; P97052, NHAB_PSEPU; P13449, NHAB_RHOER; Q53117, NHAB_RHOSO; P21220, NHB1_RHORH; P29379, NHB2_RHORH;

View entry in original ENZYME format

If you would like to retrieve all the SWISS-PROT entries referenced in this entry, click here.

NiceZyme View of ENZYME: EC 3.5.1.4

Official Name

Amidase.

Alternative Name(s)

Acylamidase.
Acylase.

Reaction catalysed

```
    A monocarboxylic acid amide
 +  H(2)O
<=>
    a monocarboxylate
 +  NH(3)
```

Cross-References

PROSITE	PDOC00494
BRENDA	3.5.1.4
EMP/PUMA	3.5.1.4
WIT	3.5.1.4
KYOTO UNIVERSITY LIGAND CHEMICAL DATABASE	3.5.1.4
IUBMB Enzyme Nomenclature	3.5.1.4
MEDLINE	Find literature relating to 3.5.1.4
SWISS-PROT	P11436, ALAM_PSEAE; Q01360, ALAM_RHOER; P08158, AMDS_EMENI; P22580, AMDY_YEAST; O05835, AMI1_MYCTU; Q11056, AMI2_MYCTU; O33040, AMI3_MYCLE; Q10811, AMI3_MYCTU; O50404, AMI4_MYCTU; P27765, AMID_PSECL; O69768, AMID_PSEPU; P22984, AMID_RHOER; P95896, AMID_SULSO; Q55424, AMID_SYNY3; O28325, YJ54_ARCFU;

View entry in original ENZYME format
If you would like to retrieve all the SWISS-PROT entries referenced in this entry, click here.

Journal of Molecular Catalysis B: Enzymatic
Volume 6, Issue 3, 11 March 1999, Pages 249-256

PII: S1381-1177(98)00080-0

A new enzymatic method of nitrile synthesis by *Rhodococcus* sp. strain YH3-3[1]

ILL

Yasuo Kato, Ryoko Ooi and Yasuhisa Asano*

Biotechnology Research Center, Faculty of Engineering, Toyama Prefectural University, 5180 Kurokawa, Kosugi, Toyama 939-0398, Japan

Received 6 February 1998; accepted 3 March 1998. Available online 10 January 2000.

Abstract

The substrate specificity of a novel aldoxime dehydratase from *E*-pyridine-3-aldoxime assimilating bacterium, *Rhodococcus* sp. strain YH3-3, was examined. The enzyme catalyzed a dehydration reaction of various aryl- and alkyl-aldoximes to form the corresponding nitriles, but did not act on arylalkyl- and substituted alkyl-aldoximes. Of various aldoximes tested, *E*-pyridine-3-aldoxime was the most suitable substrate for the enzyme. *E*-Pyridine-3-aldoxime analogs such as *O*-acetyl-*E*-pyridine-3-aldoxime, *Z*-pyridine-3-aldoxime, and *E*/*Z*-pyridine-3-aldehyde-hydrazone also acted as substrates and were converted to 3-cyanopyridine. Heat-treatment of the cells increased the accumulation of 3-cyanopyridine from *E*-pyridine-3-aldoxime because the nitrile degrading enzyme, nitrile hydratase was inactivated. Under the optimized reaction conditions (pH 7.0, 30°C), various nitriles were synthesized from the corresponding aldoximes in preparative scales with heat-treated cells of the strain. This is the first report on the microbial synthesis of nitriles from aldoximes.

- microorg inherently has activity of cyano → carboxyl

Author Keywords: Enzymatic synthesis; Aldoxime; Nitrile; Oxime dehydratase; *Rhodococcus* sp.; Screening

[1]Dedicated to Professor Hideaki Yamada in honor of his 70th birthday.

*Corresponding author. Tel.: +81-766-567500, ext. 530; fax: +81-766-562498; e-mail: asano@pu-toyama.ac.jp.

Journal of Molecular Catalysis B: Enzymatic
Volume 6, Issue 3, 11 March 1999, Pages 249-256

This Document
▸ Abstract
· Full Text + Links
· PDF (124 K)

Actions
· E-mail Article

11 of 27 results list | previous | next

=> d fall hit 2

L10 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:120991 HCAPLUS
DOCUMENT NUMBER: 130:295593
TITLE: A new enzymic method of nitrile synthesis by Rhodococcus sp. strain YH3-3
AUTHOR(S): Kato, Yasuo; Ooi, Ryoko; Asano, Yasuhisa
CORPORATE SOURCE: Biotechnology Research Center, Faculty of Engineering, Toyama Prefectural University, Kosugi, Toyama, 939-0398, Japan
SOURCE: Journal of Molecular Catalysis B: Enzymatic (**1999**), 6(3), 249-256
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 16-5 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7

ABSTRACT:
The substrate specificity of a novel aldoxime dehydratase from E-pyridine-3-aldoxime assimilating **bacterium**, Rhodococcus sp. strain YH3-3, was examd. The enzyme catalyzed a dehydration reaction of various aryl- and alkyl-aldoximes to form the corresponding nitriles, but did not act on arylalkyl- and substituted alkyl-aldoximes. Of various aldoximes tested, E-pyridine-3-aldoxime was the most suitable substrate for the enzyme. E-Pyridine-3-aldoxime analogs such as O-acetyl-E-pyridine-3-aldoxime, Z-pyridine-3-aldoxime, and E/Z-pyridine-3-aldehyde-hydrazone also acted as substrates and were converted to 3-cyanopyridine. Heat-treatment of the cells increased the accumulation of 3-cyanopyridine from E-pyridine-3-aldoxime because the nitrile degrading enzyme, **nitrile hydratase**, was **inactivated**. Under the optimized reaction conditions (pH 7.0, 30.degree.C), various nitriles were synthesized from the corresponding aldoximes in preparative scales with heat-treated cells of the strain. This is the first report on the microbial synthesis of nitriles from aldoximes.

SUPPL. TERM: nitrile manuf Rhodococcus
INDEX TERM: Oximes
ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(new enzymic method of nitrile synthesis by Rhodococcus)
INDEX TERM: Rhodococcus
(new enzymic method of nitrile synthesis from aldoximes by Rhodococcus)
INDEX TERM: Nitriles, preparation
ROLE: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(new enzymic method of nitrile synthesis from aldoximes by Rhodococcus)
INDEX TERM: 203210-76-8, Aldoxime dehydratase
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(in new enzymic method of nitrile synthesis from aldoximes by Rhodococcus)
INDEX TERM: 100-54-9P, 3-Cyanopyridine 109-74-0P, n-Butyronitrile 617-90-3P, 2-Furonitrile 19847-12-2P, Cyanopyrazine 25550-23-6P, Anisonitrile
ROLE: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(new enzymic method of nitrile synthesis from aldoximes by Rhodococcus)
INDEX TERM: 110-69-0, n-Butyraldoxime 620-03-1 1193-96-0 1193-99-3 3717-15-5 3717-19-9 3717-21-3 3717-24-6 26364-02-3, Pyridine-3-carboxaldehyde hydrazone 40747-04-4 51892-16-1 74231-55-3 87641-61-0 144605-36-7
ROLE: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(new enzymic method of nitrile synthesis from aldoximes

by Rhodococcus)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Asano, Y; Agric Biol Chem 1982, V46, P1165 HCAPLUS
(2) Asano, Y; Agric Biol Chem 1982, V46, P1183 HCAPLUS
(3) Asano, Y; Angew Chem Int Ed Engl 1989, V28, P450
(4) Asano, Y; Biosci Biotechnol Biochem 1994, V58, P223 HCAPLUS
(5) Botteghi, C; Synth Commun 1982, V12, P25 HCAPLUS
(6) Boucher, J; Biochemistry 1994, V33, P7811 HCAPLUS
(7) DeMaster, E; J Org Chem 1992, V57, P5074 HCAPLUS
(8) Fenselau, A; J Org Chem 1970, V35, P3546 HCAPLUS
(9) Foley, H; J Chem Soc Chem Commun 1973, P628 HCAPLUS
(10) Kato, Y; J Mol Catal B: Enzymatic 1996, V1, P151 HCAPLUS
(11) Kato, Y; to be published in Arch Microbiol
(12) Maruoka, K; Comprehensive Organic Synthesis 1991, V6, P763
(13) Saednya, A; Synthesis 1983, P748 HCAPLUS
(14) Sosnovsky, G; Synthesis 1978, P703 HCAPLUS
(15) Tagawa, Y; Heterocycles 1992, V34, P1605 HCAPLUS
(16) Whitesides, G; Angew Chem Int Ed Engl 1985, V24, P617
(17) Yamada, H; Angew Chem Int Ed Engl 1988, V27, P622

SO Journal of Molecular Catalysis B: Enzymatic (**1999**), 6(3), 249-256
CODEN: JMCEF8; ISSN: 1381-1177

AB The substrate specificity of a novel aldoxime dehydratase from E-pyridine-3-aldoxime assimilating **bacterium**, Rhodococcus sp. strain YH3-3, was examd. The enzyme catalyzed a dehydration reaction of various aryl- and alkyl-aldoximes to form the corresponding nitriles, but did not act on arylalkyl- and substituted alkyl-aldoximes. Of various aldoximes tested, E-pyridine-3-aldoxime was the most suitable substrate for the enzyme. E-Pyridine-3-aldoxime analogs such as O-acetyl-E-pyridine-3-aldoxime, Z-pyridine-3-aldoxime, and E/Z-pyridine-3-aldehyde-hydrazone also acted as substrates and were converted to 3-cyanopyridine. Heat-treatment of the cells increased the accumulation of 3-cyanopyridine from E-pyridine-3-aldoxime because the nitrile degrading enzyme, **nitrile hydratase**, was **inactivated**. Under the optimized reaction conditions (pH 7.0, 30.degree.C), various nitriles were synthesized from the corresponding aldoximes in preparative scales with heat-treated cells of the strain. This is the first report on the microbial synthesis of nitriles from aldoximes.